PHYS3022 APPLIED QUANTUM MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 1 EXERCISE CLASSES (6-10 January 2020)

TA will discuss the **SAMPLE QUESTIONS** in exercise classes every week. The Sample Questions are designed to serve several purposes. They served as worked example. They also review what you have learnt in previous courses that are needed in AQM, tell a physics story, enrich discussions in lectures, and some are *closed related* to the questions in an upcoming Problem Set. Students should be able to do the homework problems independently after attending the exercise class. **You should attend one exercise class session.** You are encouraged to work out (or at least think about) the sample questions before attending exercise class and ask the TA questions. Over the semester, you are welcome to go to the TAs for help.

SQ1 - $Y_{1,1}$, $Y_{1,-1}$ and p_x, p_y (QM is physics, math, and chemistry beautifully combined)
SQ2 - Atomic spectrum or spectroscopy is key to quantum physics developments
SQ3 - Free information on what's happening at the frontiers of physics

SQ1 *$Y_{1,1}$, $Y_{1,-1}$ and p_x, p_y* (QM is physics, math, and chemistry beautifully combined)

In solving QM spherically symmetric problems, we got $Y_{\ell m_\ell}(\theta,\phi)$. The spherical harmonics could be complex and the pictures of them (google them) do not often resemble those atomic orbitals you saw in chemistry courses, but they are related. For example, (Click here on soft copy for some pictures of spherical harmonics as given by the Mathematica site)

(a) While $Y_{1,0}$ can readily be shown to be related to the p_z orbital in atomic physics, the other two $Y_{1,1}$ and $Y_{1,-1}$ for $\ell = 1$ don't look like p_x and p_y at all. Even worse, they are complex! TA: **Illustrate** that, for example, $|Y_{1,1}(\theta,\phi)|^2$ and $|Y_{1,-1}(\theta,\phi)|^2$ (by a picture) don't resemble anything related to p_x and p_y (i.e., ∞-shaped pointing in x and y directions). Then, **show clearly that** combinations of $Y_{1,1}$ and $Y_{1,-1}$, i.e., $\sim (Y_{1,1} \pm Y_{1,-1})$, give the *real* p_x and p_y orbitals, which have the same shape as p_z but directed in the x and y different directions, respectively.

(b) In quantum physics, the Spherical Harmonics Y_{ℓ,m_ℓ} enters the scene as the solutions to the angular part of the Schrödinger equation for $U(r)$ (spherically symmetric) problems and H-atom in particular. Y_{ℓ,m_ℓ} are also eigenstates of $\hat{L}^2$ (magnitude squared of orbital angular momentum) and $\hat{L}_z$ (z-component of orbital angular momentum) with $\hat{L}^2 Y_{\ell,m_\ell} = (\ell(\ell+1)\hbar^2)Y_{\ell,m_\ell}$ and $\hat{L}_z Y_{\ell,m_\ell} = (m_\ell \hbar)Y_{\ell,m_\ell}$.

TA: **Illustrate** whether the p_x combination (which is a function of θ and ϕ) is an eigenstate of $\hat{L}^2$ or not. **Check it also for $\hat{L}_z$.**

(c) Spherical harmonics Y_{ℓ,m_ℓ} with different indices are orthogonal, as defined through an integral (see class notes). The orthogonality among p_x, p_y, and p_z seem natural and intuitive, as they really point at different directions that make an angle of 90° to each other. TA: From the definitions of p_x and p_y, **show that** they are indeed mathematically orthogonal to each other, using the orthogonality property of spherical harmonics.

(d) The same trick also works to define real functions from complex ones for $\ell = 2$ (d orbitals). For example, try to linearly combine $Y_{2,1}$ and $Y_{2,-1}$ to form two real functions.

[Remark: There are five real d-states often used in chemistry and solid state physics and they are orthogonal to each other. They come from linearly combining Y_{2,m_ℓ}, with $m_\ell = -2, -1, 0, +1, +2$ in suitable ways.]

SQ2 *Atomic spectrum or spectroscopy is key to quantum physics developments*

Background - Physics is an **experimental science** and its developments are often driven by experimental observations and measurements of increasing precision. Atomic and moelcular spectroscopy (seeing "light" (EM waves or photons) being absorbed or emitted) had led to key developments in quantum mechanics. The Balmer series of hydrogen spectrum was known in the 19th century. Rydberg played with the known data at the time including Balmer and the other series and came up with a description that the energy correspondence of the spectral lines are given by differences of terms of the form $\sim -\frac{1}{n^2}$. Bohr took it as a statement of the conservation of energy and then came up with the Bohr's model in 1913. Einstein put together Bohr's model and Planck's black-body radiation formula and came up with the idea of stimulated emission and thus laser (to be discussed in the course). Heisenberg wanted to explain the observed intensities of the spectral lines and founded his matrix version of quantum mechanics. Schrödinger wanted to replace the ad hoc rule that Bohr imposed (quantizing the orbital angular momentum to $n\hbar$) by the more natural boundary conditions that matter wave functions ought to be properly behave (continuous, single-valued, can be normalized, etc.) and came up with the time-independent Schrödinger equation in 1926. As spectrometer became more precise, what regarded as one spectral line in the past often came up to be two closely-spaced lines – **fine structure**. Highly accurate spectroscopy in the 20th century had further revealed the hyper-fine structure, and the Lamb shift that eventually led to the development of quantum electrodynamics (QED) - the first successful quantum field theory. All these are only about the hydrogen atom. Many more useful applications were developed when precision spectroscopy was applied to other atoms and molecules. The first thing to realize is – **we should show great respect towards good experimentalists!** Two Nobel Chemistry Prizes in the past 4 years (2014 and 2017) were also awarded for clever manipulation of light in high-resolution microscopy.

(a) The simplest version of the Bohr model or solving the Schrödinger equation for a hydrogen atom with the proton fixed at the origin gives the energies of a hydrogen atom as

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2}\frac{1}{n^2} \qquad n = 1, 2, \ldots \tag{1}$$

or you might have seen this in terms of $\hbar$ instead of h. Here, m is the mass of an electron. First, **we learn to speak the spectroscopists' language**. **Show that** the related **wave number** $\overline{\nu}$ that has the units of cm^{-1} is given by

$$\overline{\nu} = \frac{me^4}{8\epsilon^2 ch^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \tag{2}$$

for a transition between n_1 and n_2 levels. **Evaluate** R_H the limiting value that the electron just becomes detached from the nucleus (ionized) in units of cm^{-1}. The value turns out to be 109,7xx cm^{-1}.

(b) Precision spectroscopy gives us many data. The National Institute of Standards and Technology (NIST) of USA has measured, updated, and published data for various atomic transitions to very high accuracy. The NIST site http://www.nist.gov/pml/data/handbook/index2.cfm (Click here on soft copy to link to site) has many data. You could select "element name" and then "hydrogen" and you will see some atomic data. Then select "energy levels", you will see accurate data of the hydrogen energy levels as measured as absorption and emission. (Click here on soft copy to link to page) Take the limiting value from data and discuss the discrepancy in view of replacing the electron mass by the reduced mass, i.e., taking into account of the fact that the hydrogen atom problem is actually a two-body problem.

[Remarks: In class notes on the Quantum Theory of the Hydrogen Atom, it is further illustrated that there is a tiny discrepancy between the results of E_n (depends on n only) and spectroscopic data. For example, $2s$ and $2p$ have slightly different energies. Investigating the physics behind this discrepancy had led to profound concepts, e.g. spin-orbit interaction. In addition, you should appreciate that scientists are constantly making efforts in measuring quantities more accurately, and data bases are constantly updated.]

SQ3 *Free information on what's happening at the frontiers of physics*

What are the breakthroughs in physics in 2019? What's new in physics this week? TA will show you a few physics-related websites that provide free-of-charge weekly update on the latest hot topics and papers in physics. They include the American Physical Society that issues physics alerts (go to https://physics.aps.org/ or click on soft copy here), and the Institute of Physics in UK provides weekly alerts under physicsworld.com (newswire). Students are encouraged to register (free of charge) and receive weekly updates on what's hot in physics. This is a step in bringing yourself closer to real physics and going beyond textbook physics.

For example, (click here on soft copy to go to physicsword site by Institute of Physics UK or go to https://physicsworld.com/)

The international journals *Nature* and *Science* also provide weekly alerts on the latest developments in science (not only physics). Even BBC news provides updates on science and the environment.